Summer Project on Condensed Matter Physics - IISc, Bangalore 2023

Lecture 7: Graphene

22nd May, 2023

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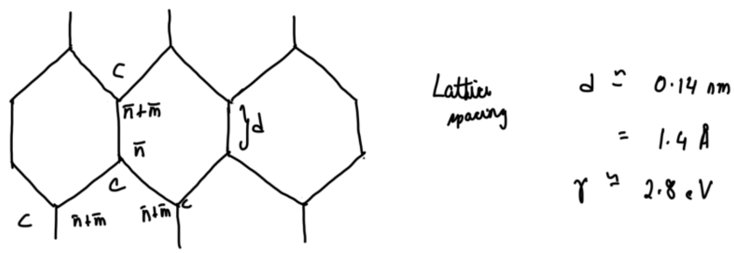
The structure of graphene was understood and the eigenvalue problem for graphene was solved.

1 Graphene Structure



If we label a particular lattice site with position vector $\vec{n}$, then a adjacent lattice point will be labelled by $\vec{n}+\vec{m}$.
Then, the Hamiltonian will be written as:

$$H = -\gamma \sum_{\vec{n},\vec{m}} [c^{\dagger}_{\vec{n}} c_{\vec{n}+\vec{m}} + c^{\dagger}_{\vec{n}+\vec{m}} c_{\vec{n}}] \tag{1}$$

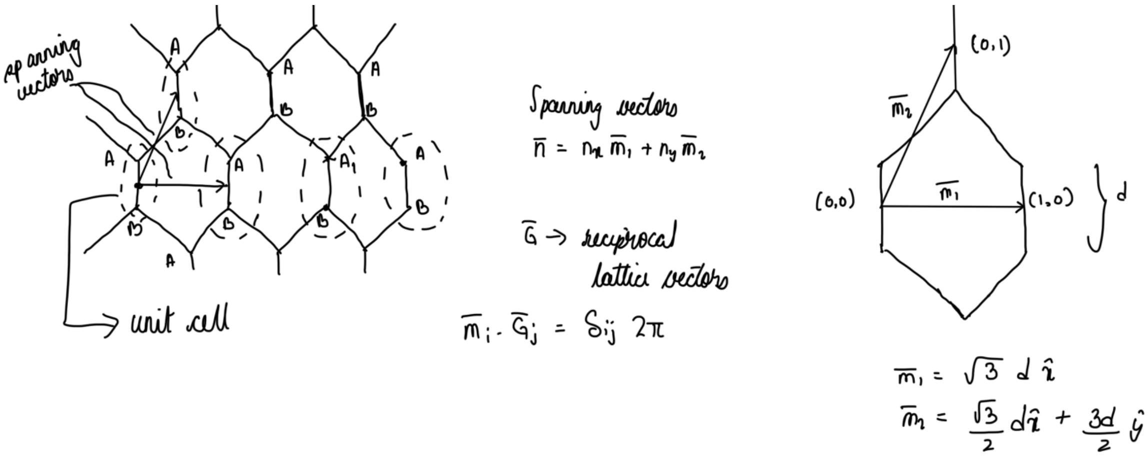
In general, we ca define a creation operator $c^{\dagger}_{\vec{m},\sigma}$ which creates one electron at site m with spin σ. The creation and annhilation operators satisfy the following anticommutator relations:

$$\{c_{\vec{m},\sigma}, c_{\vec{n},\sigma'}\} = 0 \tag{2}$$

$$\{c_{\vec{m},\sigma}, c^{\dagger}_{\vec{n},\sigma'}\} = \delta_{mn}\delta\sigma\sigma' \tag{3}$$

1.1 Triangular Lattice

Clearly, graphene structure is not a Bravais lattice but is actually a honeycomb lattice. The graphene structure can be thought of as a triangular lattice with a basis. Equivalently, we consider a unit cell containing two atoms as shown in the diagram. The two atom sites in the unit cell can e labelled by A and B.



The spanning vectors of this lattice can be written in terms of two lattice translational vectors, let's call them $\vec{m_1}$ and $\vec{m_2}$. Then,

$$\vec{m_1} = \sqrt{3} d\hat{x} \tag{4}$$

$$\vec{m_2} = \frac{\sqrt{3}}{2} d\hat{x} + \frac{3}{2} d\hat{y} \tag{5}$$

Correspodningly, we can define reciprocal lattice vectors which satisfy $\vec{m_i}.\vec{G_j} = \delta_{ij} 2\pi$:

$$\vec{G_1} = \frac{2\pi}{\sqrt{3}d}\hat{x} - \frac{2\pi}{3d}\hat{y} \tag{6}$$

$$\vec{G_2} = \frac{4\pi}{3d}\hat{y} \tag{7}$$

2 States and Energies

Since, we are now in two-dimensions, we will need two components of wave vector to label electron states. Thus we can write an electron state as:

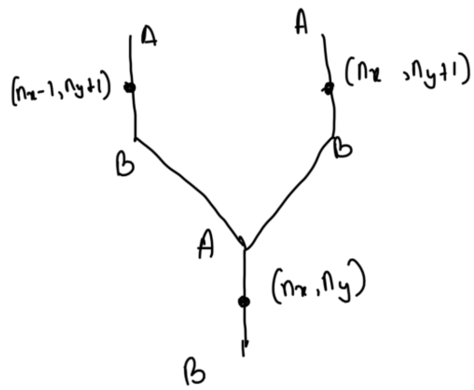
$$|\vec{k}\rangle = |k_x, k_y\rangle = \sum_{n_x, n_y} [|A(G_x, G_y\rangle + |B(G_x, G_y\rangle] e^{(k_x n_x + k_y n_y)d} \tag{8}$$

where, $|A\rangle$ and $|B\rangle$ refer to the state of an electron to be at lattice site A and B respectively:

$$|A(n_x, n_y)\rangle = |\alpha\rangle\, e^{(k_x n_x + k_y n_y)d} \tag{9}$$

$$|B(n_x, n_y)\rangle = |\beta\rangle\, e^{(k_x n_x + k_y n_y)d} \tag{10}$$

Next, we can label particular lattice sites with indices n_x and n_y as shown below.



Just like in the SSH model we can act the Hamiltonian on these states to get the following equations:

$$E\left|\alpha\right\rangle = -\gamma\left|\beta\right\rangle - \gamma\left|\beta\right\rangle e^{ik_yd} - \gamma\left|\beta\right\rangle e^{-ik_xd+ik_yd} \tag{11}$$

$$E\left|\beta\right\rangle = -\gamma\left|\alpha\right\rangle - \gamma\left|\alpha\right\rangle e^{ik_yd} - \gamma\left|\beta\right\rangle e^{ik_xd-ik_yd} \tag{12}$$

$$\begin{pmatrix} 0 & -\gamma-\gamma e^{ik_yd}-\gamma e^{-ik_xd+ik_yd} \\ -\gamma-\gamma e^{-ik_yd}-\gamma e^{-ik_xd-ik_yd} & 0 \end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = E\begin{pmatrix}\alpha \\ \beta\end{pmatrix} \tag{13}$$

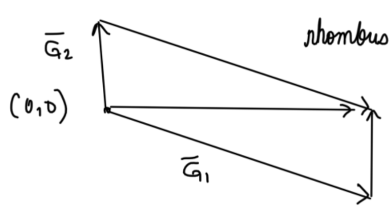
Eigenvalues of $\begin{pmatrix} 0 & c \\ c* & 0\end{pmatrix} = \lambda \pm |c|$

$$\begin{aligned}\lambda &= \pm(\gamma^2+\gamma^2e^{ik_yd}+\gamma^2e^{-ik_xd+ik_yd}+\gamma^2e^{-ik_yd}+\gamma^2e^{-ik_xd}+\gamma^2e^{ik_xd-ik_yd}+\gamma^2e^{ik_xd}+m\gamma^2)^{\frac{1}{2}} \\ &= \pm(3\gamma^2+2cos(k_yd)+2\gamma^2cos(k_xd)+2\gamma^2cos(k_xd-k_yd))^{\frac{1}{2}} \\ \lambda &= \pm|\gamma|(3+2cos(k_yd)+2cos(k_xd)+2cos(k_xd-k_yd))^{\frac{1}{2}}\end{aligned}$$

Energies:

$$E = \pm|\gamma+\gamma e^{ik_yd}+\gamma e^{ik_xd+ik_yd}| \tag{14}$$

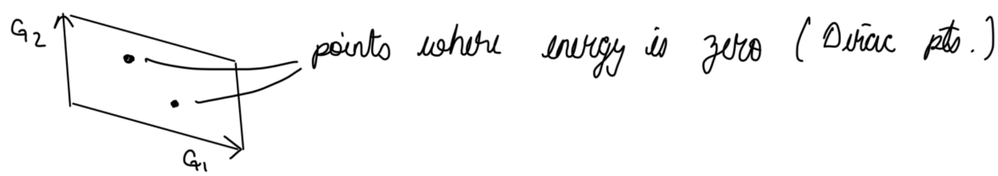
$$= \gamma|1+e^{ik_yd}+e^{-ik_xd}| \tag{15}$$

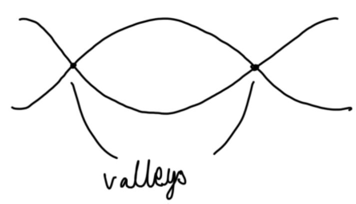


Translational vectors: $\vec{n} = n_x \vec{m}_1 + n_y \vec{m}_2$
Wave vector: $\vec{k} = k_x \vec{G}_1 + k_y \vec{G}_2$

$$\vec{k} \cdot \vec{n} = k_x n_x + k_y n_y$$

Points where energy is zero are: $\left(\frac{4\pi}{3\sqrt{3}d}, 0\right)$ and $\left(\frac{-4\pi}{3\sqrt{3}d}, 0\right)$ in the $\hat{x}, \hat{y}$ basis.





$$\vec{k} = \left(\frac{4\pi}{3\sqrt{3}d}, 0\right) + (\delta k_x, \delta k_y) \rightarrow \text{k valley}$$
$$\vec{k'} = \left(\frac{-4\pi}{3\sqrt{3}d}, 0\right) + (\delta k_x, \delta k_y) \rightarrow \text{k' valley}$$

$$\text{Near a k valley: } H = \frac{3\gamma d}{2}(\delta k_x \sigma^x + \delta k_y \sigma^y) \tag{16}$$
$$= \frac{3\gamma d}{2}\begin{pmatrix} 0 & \delta k_x - i\delta k_y \\ \delta k_x + i\delta k_y & 0 \end{pmatrix} \tag{17}$$

$$\text{Near a k' valley: } H = \frac{3\gamma d}{2}(-\delta k_x \sigma^x + \delta k_y \sigma^y) \tag{18}$$
$$= \frac{3\gamma d}{2}\begin{pmatrix} 0 & \delta - k_x - i\delta k_y \\ \delta - k_x + i\delta k_y & 0 \end{pmatrix} \tag{19}$$

So,we write the state as:

$$\psi(n_x, n_y) = e^{i\vec{k_0}\cdot\vec{n}}\psi_k(n_x, n_y) + e^{-i\vec{k_0}\cdot\vec{n}}\psi_{k'}(n_x, n_y) \tag{20}$$

where,

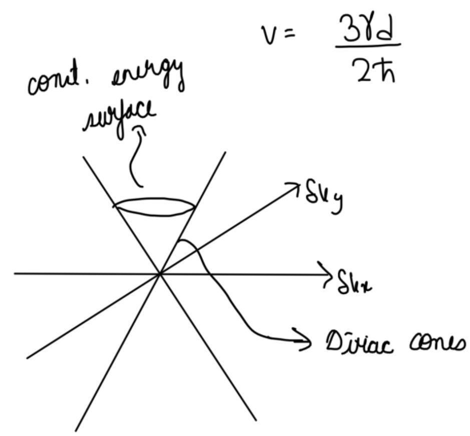
$$\psi_k \to e^{i(\delta k_x \hat{x} + \delta k_y \hat{y})\cdot \vec{n}} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

The above state satisfies:

$$H = \frac{3\gamma d}{2}\left(\sigma^x\left(-i\frac{d}{dx}\right) + \sigma^y\left(-i\frac{d}{dy}\right)\right) \tag{21}$$

The energy dispersion near a valley is of the form:

$$E = \pm\sqrt{\left(\frac{3\gamma d}{2}\right)^{\frac{1}{2}}\left(\delta k_x^2 + \delta k_y^2\right)} \tag{22}$$



In one dimension, the Dirac equation for this system will be written as:

$$i\hbar\frac{\partial\psi}{\partial t} = \left[\hbar v\left(-i\frac{\partial}{\partial x}\right)\sigma^z + V(x)\right]\psi = E\psi \tag{23}$$